Universal ionic valence velocity scaling

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This work combines the usual empirical formula for the effective charge of a beam penetrating a target with the Bohr charge equilibrium condition. The result is a logarithmic scaling law, which provides the rms valence velocity and virialized ionization potential for any atomic species Z at any charge state $0 \leq Q < Z$. Comparisons with Thomas-Fermi modeling and the Bohr formula for hydrogenic valence velocities are performed.

I. BACKGROUND

Two principal atomic modeling systems, the Bohr atom and the Thomas-Fermi model, treat atomic electron distributions in two distinct manners each, with different regimes of applicability. A bridge between the two systems can be found in an empirical formula that approximates the effective charge state of an ion beam penetrating a cold target. The nature of this formula will be investigated here in detail. In particular, combining the effective charge formula with an equilibrium charge condition due to Bohr will produce a generalized modeling scheme for valence electron energetics.

As an ion beam is deposited into a target, its constituent ions can be characterized by an average charge state that likely represents an equilibrium value at each instant of the beam's journey. The kinetic balance responsible for establishing this charge equilibrium was specified by Bohr [1]. He surmised that a beam's equilibrium ionicity at each point during its penetration into a target would be that ionic charge Q at which the rms valence electron velocity $v_v(Z,Q)$ roughly equals the beam velocity v. While providing insight into the nature of the atomic energetic balance of an incident beam, Bohr's *ansatz* does not immediately provide a way to quantify the beam's instantaneous charge state.

Apparently distinct from the Bohr condition is the use of empirical formulas that provide the effective charge state of a beam penetrating a cold target. The most common application of such formulas is to provide an effective beam charge state for energy deposition calculations. In general, a beam's instantaneous effective charge state $Q(v,Z)$ can be independent of the target species and is a function only of the beam's velocity v and atomic number Z. Owing to the work of Brown and Moak [2] is a particularly successful empirical formula for $Q(v,Z)$. It can be written as

$$Q(v,Z) \approx Z \left(1 - a \exp\left[\frac{-v}{Z^f \alpha c} \right] \right), \qquad (1)$$

where a is a parameter near unity and f is a parameter whose value is near 2/3.

The chief purpose of Eq. (1) is to provide a value for the incident ionic charge Q appearing in the Bethe formula for beam stopping power dE/dx [3]. The Bethe formula depends on the square of this charge [4]

$$\frac{dE}{dx} = \frac{-4\pi e^4 Q^2}{m_e v^2} n_b \ln[\Lambda_b], \qquad (2)$$

in which n_b is the number density of bound electrons in the target and Λ_b is the Coulomb logarithm. Brown and Moak selected $a = 1.034$ and $f = 0.69$ for an optimal form of Eq. (1) for modeling the range of incident ion beams in targets. A curious yet unaddressed detail of the fitted parameters is that

$$\frac{f}{2/3} = 1.035 \approx a. \qquad (3)$$

With the substitution $f \equiv 2b/3$ a useful interpretation of the term $Z^f \alpha c$ as the slightly corrected Thomas-Fermi velocity becomes transparent.

II. VALENCE SCALING

It was observed that the effective charge $Q(v,Z)$ given by Eq. (1) closely represented the actual average ionic charge of the beam [2]. After traversing a target and emerging at a velocity v, an ion beam exhibited an average charge that was well represented by the effective charge formula. Brown and Moak noted that this concurrence was "interesting to observe," but no substantial exploration was conducted. Suppose that the effective charge state given by Eq. (1) is indeed consistent with the equilibrium charge state imposed by the Bohr condition. In other words, the charge state given by the effective charge formula ought to be nearly the same as the charge state at which the characteristic valence velocity is equal to the beam velocity. This connection between the two models, if valid, will produce an interesting result after a simple substitution.

The Bohr charge equilibrium condition can be stated as

$$v \approx v_v(Z,Q), \qquad (4)$$

where $v_v(Z,Q)$ is the rms valence velocity of an ion of atomic number Z at a charge state Q. Exploiting the putative consistency between the Bohr model and the empirical fit of Brown and Moak, this substitution can be applied to Eq. (1) producing

$$Q \approx Z \left(1 - a \exp\left[\frac{-v_v(Z,Q)}{Z^{2b/3} \alpha c} \right] \right). \qquad (5)$$

Solving for $v_v(Z,Q)$ gives

$$v_v(Z,Q) \approx Z^{2b/3} \alpha c \ln\left[\frac{aZ}{Z-Q}\right]. \qquad (6)$$

This formula contains the bold implication of providing the rms valence electron velocity of any species Z at a charge state Q. The empirical fit for a beam's effective charge state is seen implicitly to contain generalized information about the scaling of ionic valence levels. Given the universality of the original formula in Eq. (1), the inverted form should also enjoy application to a wide range of atomic species and charge states. Furthermore, Eq. (6) can be used in principle to form a virialized ionization potential $I(Z,Q)$ of any species at any given charge state. In the nonrelativistic limit, the ionization potential can be taken from the valence rms velocity $v_v(Z,Q)$ by

$$I(Z,Q) = \frac{1}{2} m_e v_v^2(Z,Q), \qquad (7)$$

or relativistically by

$$I(Z,Q) = (1-s) m_e c^2, \qquad (8)$$

with $s^2 = 1 - [v_v(Z,Q)/c]^2$ and m_e being the electron mass [5]. The explicit form for the nonrelativistic valence ionization potential in Eq. (7) is

$$I(Z,Q) \approx Z^{4b/3} \text{Ry} \left(\ln\left[\frac{aZ}{Z-Q}\right] \right)^2, \qquad (9)$$

with $\text{Ry} \equiv \frac{1}{2} m_e \alpha^2 c^2$.

A. Calculations with the scaling

The information provided by the general yet surprisingly compact forms of Eqs. (6)–(9) will be applied to several cases to investigate the value of these alleged relationships. In the following calculations, the parameter a will be set to 1.034, the value chosen by Brown and Moak. The value of b will be set to unity throughout, maintaining the presence of the unadjusted Thomas-Fermi velocity in the equations. Figure 1 displays the rms valence electron velocities for lead and silver for each of their respective charge states extracted from the measured ionization potentials. Also shown are the valence velocities calculated from Eq. (6). Aside from shell effects, the scaling of the measured valence velocities with charge state is represented with impressive reliability.

Figure 2 displays the measured ionization potentials of lead for all charge states along with the ionization potentials calculated with the logarithmic scaling. Across approximately four orders of magnitude of energies, Eqs. (6)–(9) well reproduce the measured ionization potentials, in both relativistic and nonrelativistic regimes. Note the importance of the a parameter in Fig. 2. At low charge states the value of a influences the logarithmic numerator and noticeably increases the calculated ionization potential compared to calculations with $a=1$.
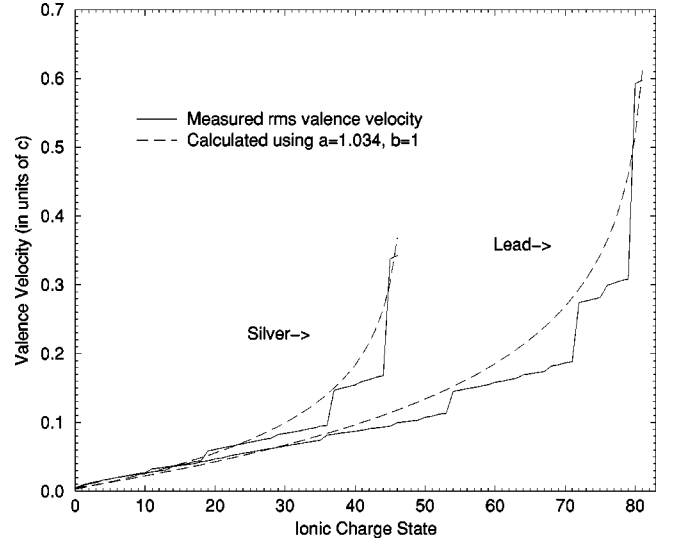

FIG. 1. Calculated and measured rms valence velocities for all charge states of silver and lead.

III. COMPARISON TO THOMAS-FERMI MODELS

The Thomas-Fermi (TF) treatment of atomic and ionic energetics can be used to model the scaling of ionization potential with charge state. The results given by the TF model will be compared with the logarithmic scaling introduced here. The total TF binding energy E_{TF} of the electrons in a neutral species scales as $Z^{7/3}$ [6]. For an ionized species, this scaling is adjusted by a term $e(Z,N)$, which is a function of the degree of ionization

$$E_{TF}(Z,N) \propto Z^{7/3} e(Z,N), \qquad (10)$$

where N is the number of bound electrons and the charge state Q of the ion is $Z-N$ [7]. The ionization potential $I(Z,Q)$ of an ionic species can be determined from total electronic binding energies by
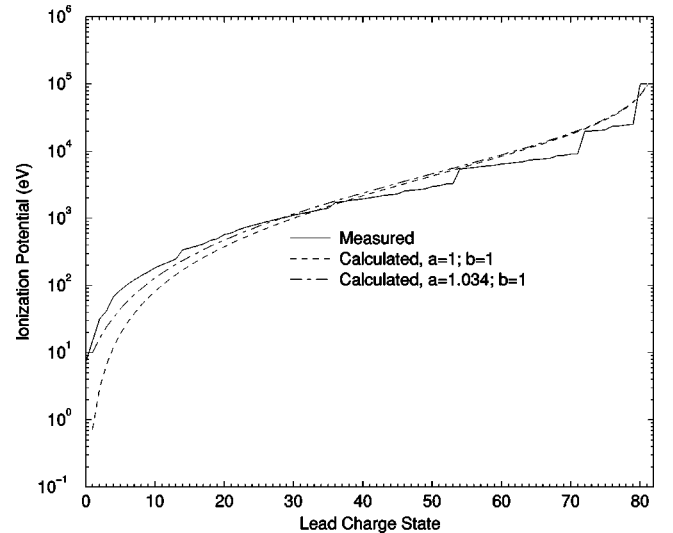

FIG. 2. Calculated and measured ionization potentials for all charge states of lead.
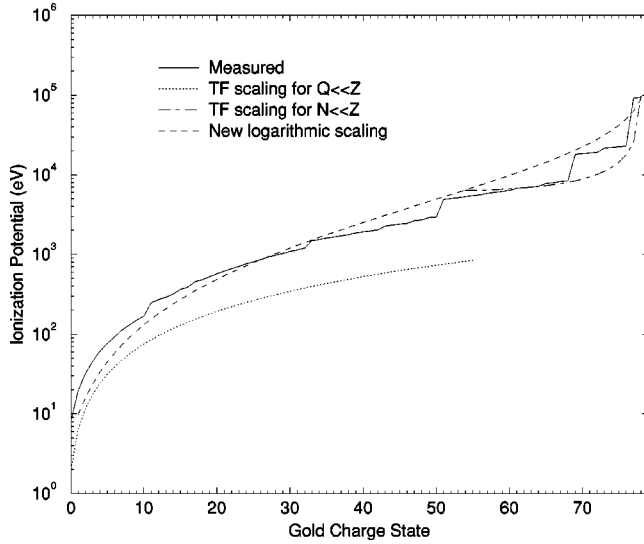
FIG. 3. Calculated and measured ionization potentials for all charge states of gold along with Thomas-Fermi modeling.

$$I(Z,Q) = E_{TF}(Z,N) - E_{TF}(Z,N-1). \tag{11}$$

In practice, the scaling function $e(Z,N)$ is not able to be stated analytically for the entire range of $0 < N \leq Z$. Analytical approximations are available for the two cases N being very close to Z and N being near unity. Following Ref. [7], for N not much less than Z (ions of low charge state $Q \ll Z$), the total binding energy scales as

$$E_{TF}(Z,N) \approx 0.769 Z^{7/3} - 0.0473(Z-N)^{7/3}, \tag{12}$$

in which the energy is given in atomic units. For $N \ll Z$ (highly charged ions) the TF binding energy is approximated by

$$E_{TF}(Z,N) \approx 1.14 Z^2 \left(\frac{3}{2}N\right)^{1/3} - 0.485 Z N^{4/3}. \tag{13}$$

By employing these expressions in Eq. (11) the ionization potential can be approximated for an arbitrarily charged species. Note that Eq. (12) will produce an ionization potential, which is a function only of $Q = Z - N$ since the leading term $0.769 Z^{7/3}$ will cancel in application of Eq. (11). Dependency on Z can be added for a better approximation by incorporating terms that are expansions of $q \equiv 1 - N/Z$ (see Ref. [7] for complete details).

Figure 3 displays the ionization potentials of gold at all charge states calculated with the Thomas-Fermi scaling. For comparison are shown the measured values and the results obtained using Eqs. (6)–(9). For high charge states $N \ll Z$ the TF model's scaling reproduces well the empirical trends. It is curious to note that the TF model follows a different trajectory along the shell structure trends than does the logarithmic scaling, yet both capture important characteristic features. The functionalities of the two models in this regime are clearly distinct, as expected from the difference between Eq. (13) and the virialized Eq. (6). At low charge states the effectiveness of the TF model suffers from the absence of ap-

propriate functional dependence on atomic number Z. The logarithmic scaling exhibits appropriate Z dependence and performs much more effectively in this regime. However, as is evident from Fig. 3, the functional variation of the two models with charge state Q are very similar. This can be understood by examining the associated formulas. Equation (12) varies roughly as the 7/3 power of Q. On the other hand, the valence velocity in Eq. (6) can be approximated for $Q \ll Z$ by

$$v_v(Z,Q) \approx Z^{2/3} \alpha c \left(\frac{Z}{Z-Q} - 1\right), \tag{14}$$

(with $a = b = 1$ for clarity). With continued reduction this gives

$$v_v(Z,Q) \approx \frac{Q \alpha c}{Z^{1/3}}. \tag{15}$$

Thus, in the low-ionicity limit, the logarithmic formula gives a valence velocity that scales linearly with Q and thus a virialized ionization potential that scales as the square of charge state, in rough agreement with the 7/3 power scaling of the TF model in this regime.

IV. HYDROGENIC CONSISTENCY AND A LOGARITHMIC RELATIONSHIP

Consider the special case of a hydrogenic ion with $Q = Z - 1$. As demonstrated in Fig. 1, Eq. (6) can be used to model the hydrogenic electron's rms velocity (see the velocities calculated for $Q = 46$ for silver and $Q = 81$ for lead). The generalized formula for the hydrogenic rms valence velocity v_h according to the logarithmic scaling is

$$v_h = v_v(Z, Q = Z-1) \approx Z^{2b/3} \alpha c \ln[aZ]. \tag{16}$$

But, a hydrogenic orbital system also should be well described by the Bohr-atom scaling in which the orbital velocity v_B varies linearly with Z,

$$v_B \approx Z \alpha c. \tag{17}$$

Are these two modeling systems consistent? If this connection between the logarithmic model and the Bohr atom should be valid, then an interesting mathematical relationship will result. Equating the hydrogenic rms valence velocities obtained by the two different methods gives, with $a = b = 1$ for clarity,

$$Z^{2/3} \alpha c \ln[Z] \approx Z \alpha c, \tag{18}$$

which is to say

$$\ln[Z] \approx Z^{1/3}. \tag{19}$$

Thus, an implication of hydrogenic consistency is an approximation to the logarithmic function. This approximation to the natural log is indeed good for Z in the range of the atomic numbers greater than a few.

V. INTERPRETATIONS AND DIRECTIONS

These previously unexplored applications of an inverted effective charge formula are perhaps most useful in the atomic scaling physics that they imply. A clear justification of the success of this logarithmic scaling from first principles is not apparent. The analyses that generated the form of Eq. (1) treated the functional development only empirically. However, the model's consistency with Bohr scaling, low-ionicity TF modeling, and measured valence energies indicate that a meaningful physical representation is being articulated.

From the consistency demonstrated here, we may also draw some conclusions about the physics of beam charge evolution. It appears that the Bohr equilibrium condition and the empirical formula of Brown and Moak are roughly equivalent statements of average beam charge state. This joins two paradigms of beam charge evolution that have generally been treated as distinct. The success of Eq. (6) reinforces the notion that the charge state provided by Eq. (1) represents an actual ionic charge and not just an effective charge parameter. This provides a more physical explanation of the success of the formula of Brown and Moak has, which been viewed simply as a fit to data.

At least one term in the empirical fit of Brown and Moak can now be interpreted not just as a fitting parameter but as representative of the physics of atomic electron distributions. The role of the parameter a accounts for the fact that the valence electrons in a neutral atom have a nonzero rms velocity. If the factor a were simply unity, Eq. (9) would give a unit argument to the logarithm and thus a vanishing ionization potential for neutral atoms ($Q=0$). Setting a to a value slightly greater than 1 corrects this trend. For higher charge states Q, the factor a becomes insignificant.

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